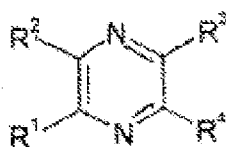


appropriate serial number.

See claims attached. Please do structure search and inventor name(s) search. Display results to show identification of source, and R¹, compound name & structure of identified compounds. Search compound of Formula I.

1. (previously presented) A compound of formula (I):



or a pharmaceutically acceptable salt thereof, in which

R¹ and R² independently represent phenyl, thienyl or pyridyl each of which is independently optionally substituted by one or more groups represented by Z;

Z represents a C₁₋₈ alkyl group optionally substituted by one or more: hydroxy; a C₁₋₆ alkoxy group optionally substituted by one or more fluoro; a C₃₋₈ cycloalkyl group; a saturated or partially unsaturated 5-to-8-membered heterocyclic group containing one or more heteroatoms selected from nitrogen, oxygen or sulphur; or by a group NR¹⁰R¹¹ (in which R¹⁰ and R¹¹ independently represent hydrogen, a C₁₋₆ alkyl group, a C₁₋₆ alkanoyl group or a C₁₋₆ alkoxy carbonyl group), or Z represents a C₃₋₈ cycloalkyl group, a C₁₋₆ alkoxy group (optionally substituted by one or more fluoro), hydroxy, halo, trifluoromethyl, trifluoromethylthio, trifluoromethylsulphonyl, nitro, a group NR¹⁰R¹¹ (in which R¹⁰ and R¹¹ independently represent hydrogen, a C₁₋₆ alkyl group, a C₁₋₆ alkanoyl group or a C₁₋₆ alkoxy carbonyl group), mono or di C₁₋₃ alkylamido, C₁₋₃ alkylthio, C₁₋₃ alkylsulphonyl, C₁₋₃ alkylsulphonyloxy, C₁₋₃ alkoxy carbonyl, carboxy, cyano, carbamoyl, mono or di C₁₋₃ alkyl carbamoyl, sulphamoyl, acetyl, an aromatic heterocyclic group which is optionally substituted by one or more halo, C₁₋₄ alkyl, trifluoromethyl or trifluoromethoxy, or Z represents a saturated or partially unsaturated 5-to-8-membered heterocyclic group containing one or more heteroatoms selected from nitrogen, oxygen or sulphur wherein the heterocyclic group is optionally substituted by one or more C₁₋₃ alkyl, hydroxy, fluoro, benzyl or an amino group -NR^xR^y in which R^x and R^y independently represent H or C₁₋₄ alkyl;

10/560862

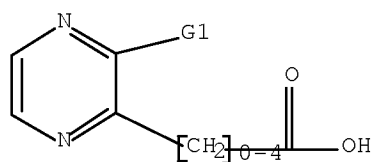
***** INVENTOR RESULTS *****

=> d his l23

(FILE 'HCAPLUS' ENTERED AT 10:35:32 ON 25 NOV 2008)
L23 4 S (L22 AND L12) OR (L12 AND L11)

=> d que l23

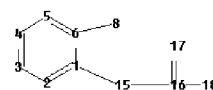
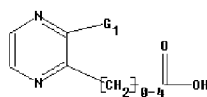
L9 STR



G1 [01], [02]

Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



chain nodes :
8 9 10 11 15 16 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-15 6-8 9-10 15-16 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
6-8 9-10
exact bonds :
1-15 15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18
isolated ring systems :

containing 1 :

G1:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS

L11 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US20070093484/PN
L12 573 SEA FILE=REGISTRY SSS FUL L9
L22 43 SEA FILE=HCAPLUS ABB=ON PLU=ON "CHENG LEIFENG"/AU
L23 4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L22 AND L12) OR (L12 AND
L11)

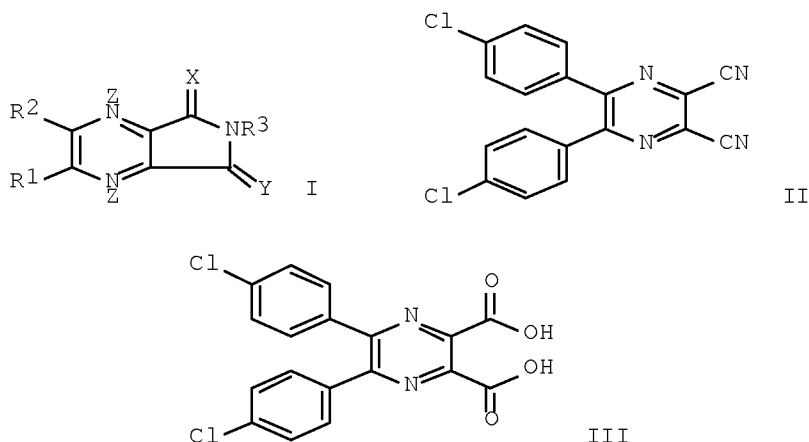
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L23 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:493608 HCAPLUS Full-text
DOCUMENT NUMBER: 143:43904
TITLE: Preparation of pyrrolo[3,4-b]pyrazine-5,7(6H)-dione
derivatives for treating obesity, psychiatric, and
neurological disorders
INVENTOR(S): Cheng, Leifeng
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051953	A2	20050609	WO 2004-GB4934	20041124
WO 2005051953	A3	20050728		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 2004292493	B2	20080124		
CA 2546318	A1	20050609	CA 2004-2546318	20041124
EP 1701958	A2	20060920	EP 2004-798641	20041124
EP 1701958	B1	20070502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS				
CN 1886405	A	20061227	CN 2004-80034802	20041124

10/560862

AT 361301	T	20070515	AT 2004-798641	20041124
JP 2007512298	T	20070517	JP 2006-540602	20041124
ES 2285544	T3	20071116	ES 2004-798641	20041124
IN 2006DN02621	A	20070824	IN 2006-DN2621	20060510
US 20070099923	A1	20070503	US 2006-579830	20060517
HK 1096670	A1	20071012	HK 2007-101236	20070201
PRIORITY APPLN. INFO.:			GB 2003-27331	A 20031125
			WO 2004-GB4934	W 20041124
OTHER SOURCE(S):		CASREACT 143:43904; MARPAT 143:43904		
GI				



AB The title compds. I [R1, R2 = Ph, thienyl, pyridyl, C1-C10-alkyl, C1-C10-alkoxy, C3-C15-cycloalkyl; R3 = C1-C15-alkyl, C3-C15-cycloalkyl, phenylC1-C4-alkyl, heteroaryl, heteroarylC1-C4-alkyl, R4(CH2)n, R4 = heterocycle, n = 0-4; X, Y = O, S; Z = (O)n, n = 0, 1] were prepared and are designed to be used in the treatment of obesity, psychiatric disorders, neurol. disorders, immune, cardiovascular, reproductive, and endocrine disorders, septic shock, diseases related to respiratory and gastrointestinal systems, and extended abuse, addiction and/or relapse indications. As an example, 1,2-bis(4-chlorophenyl)ethane-1,2-dione reacted with diaminomaleonitrile to give pyrazine-2,3-dicarbonitrile II which was treated with KOH/H2O2 in H2O, esterified, and hydrolyzed to give dicarboxylic acid III. III condensed with 4-FC6H4CH2NH2 to give the mono-amide which cyclized to give the desired compound I (R1 = R2 = 4-ClC6H4, R3 = 4-FC6H4CH2, X = Y = O, Z = none).

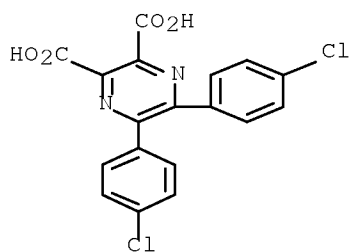
IT 810685-49-5P, 5,6-Bis(4-chlorophenyl)pyrazine-2,3-dicarboxylic acid 811441-51-7P, 5,6-Bis(4-chlorophenyl)-3-[(piperidin-1-ylamino)carbonyl]pyrazine-2-carboxylic acid 853578-19-5P 853578-23-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrrolo[3,4-b]pyrazine-5,7(6H)-dione derivs. for treating obesity, psychiatric, neurol., immune, cardiovascular, reproductive, and endocrine disorders, septic shock, respiratory and gastrointestinal disorders)

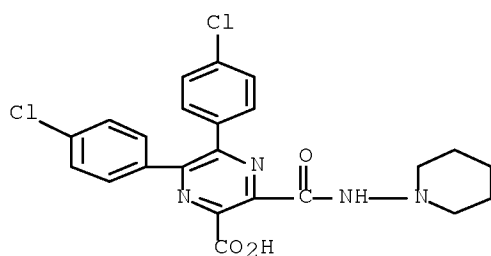
RN 810685-49-5 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)- (CA INDEX NAME)



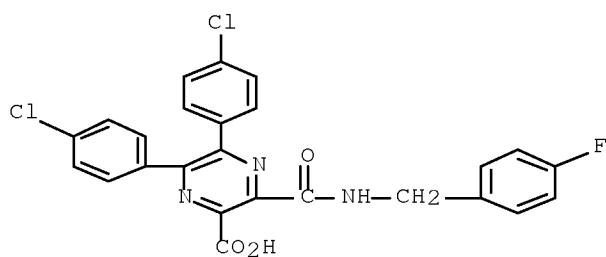
RN 811441-51-7 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 5,6-bis(4-chlorophenyl)-3-[(1-piperidinylamino)carbonyl]- (CA INDEX NAME)



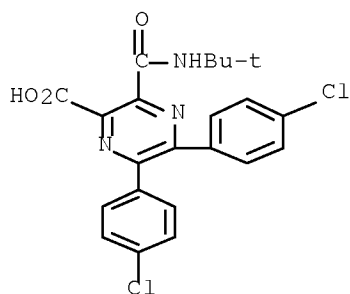
RN 853578-19-5 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 5,6-bis(4-chlorophenyl)-3-[[[(4-fluorophenyl)methyl]amino]carbonyl]- (CA INDEX NAME)



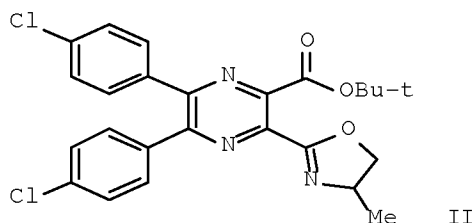
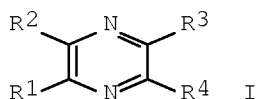
RN 853578-23-1 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 5,6-bis(4-chlorophenyl)-3-[[[(1,1-dimethylethyl)amino]carbonyl]- (CA INDEX NAME)

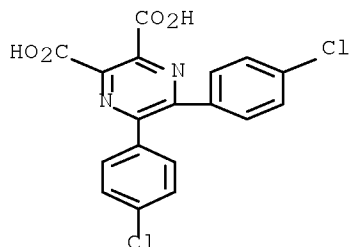


L23 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:1127371 HCAPLUS Full-text
 DOCUMENT NUMBER: 142:56364
 TITLE: Preparation of 2,3-substituted 5,6-diaryl-pyrazine derivatives as CB1 modulators
 INVENTOR(S): Cheng, Leifeng; Wilstermann, Michael
 PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
 SOURCE: PCT Int. Appl., 54 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004111039	A1	20041223	WO 2004-SE968	20040616
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004247614	A1	20041223	AU 2004-247614	20040616
AU 2004247614	B2	20080228		
CA 2527037	A1	20041223	CA 2004-2527037	20040616
EP 1638956	A1	20060329	EP 2004-749010	20040616
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2006527769	T	20061207	JP 2006-517042	20040616
US 20070093505	A1	20070426	US 2005-561033	20051216
PRIORITY APPLN. INFO.:			GB 2003-14261	A 20030619
			WO 2004-SE968	W 20040616
OTHER SOURCE(S):			MARPAT 142:56364	
GI				

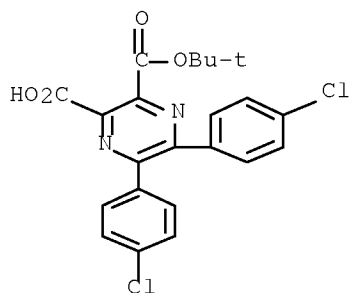


- AB Title compds. I [wherein R1, R2 = independently (un)substituted Ph, thienyl, pyridinyl; R3, R4 = (CH₂)_nCO₂R₇, CH₂OCH₂R₈, (CH₂)_qR₉ with proviso, (un)substituted alkyl, etc.; R₇ = (un)substituted cycloalkyl/cyclo/alkyl, (CH₂)_aphenyl, (un)saturated heterocyclyl; a = 0-4; R₈ = (un)substituted alkyl, Ph, (un)saturated aromatic heterocyclyl; n = 0-4; q = 0-4; R₉ = (un)substituted cycloalkyl, ph, aromatic heterocyclyl, saturated or partially unsatd. 5-12-membered heterocyclyl; and pharmaceutically acceptable salts thereof] were prepared as cannabinoid 1 (CB1) receptor modulators. Thus, reacting (DL)-alaninol with 5,6-Bis(4-chlorophenyl)-3-(tert-butoxycarbonyl)pyrazine-2-carboxylic acid (preparation given), followed by cyclization gave pyrazine II. I are active at the CB1 receptor (IC₅₀ < 1 μM), most preferred compds. have IC₅₀ < 200 nM. For instance, II exhibited an IC₅₀ (hCB1) = 1.8 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of obesity, psychiatric and neurol. disorders (no data).
- IT 810685-49-5P, 5,6-Bis(4-chlorophenyl)pyrazine-2,3-dicarboxylic acid 811436-88-1P, 5,6-Bis(4-chlorophenyl)-3-(tert-butoxycarbonyl)pyrazine-2-carboxylic acid
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of 2,3-substituted 5,6-diaryl-pyrazines as CB1 modulators)
- RN 810685-49-5 HCAPLUS
- CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)- (CA INDEX NAME)



10/560862

RN 811436-88-1 HCAPLUS
 CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)-,
 2-(1,1-dimethylethyl) ester (CA INDEX NAME)

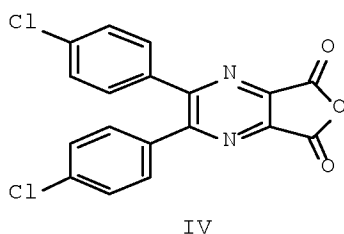
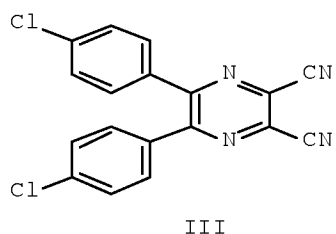


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:1127370 HCAPLUS Full-text
 DOCUMENT NUMBER: 142:56363
 TITLE: Preparation of
 5,6-bis(4-chlorophenyl)-N-piperidin-1-yl-3-(piperidin-
 1-ylcarbonyl)pyrazine-2-carboxamide for treatment of
 obesity
 INVENTOR(S): Cheng, Leifeng
 PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
 SOURCE: PCT Int. Appl., 24 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004111038	A1	20041223	WO 2004-SE967	20040616
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: GB 2003-14049 A 20030618
 GI



AB 5,6-Bis(4-chlorophenyl)-N-piperidin-1-yl-3-(piperidin-1-yl- carbonyl)pyrazine-2-carboxamide (I) was prepared by reacting 4-ClC₆H₄CHO with NaCN/EtOH which gave 1,2-bis(4-chlorophenyl)-2-hydroxyethanone (II). II was oxidized to the ethane-1,2-dione which was condensed with diaminomaleonitrile to give pyrazine III. III was converted to the corresponding 2,3-dicarboxylic acid which was treated with AcCl to give furo[3,4-b]pyrazine-5,7-dione IV. IV was then subsequently reacted with piperidine/MeCN and oxalyl chloride/1-piperidinamine/CH₂Cl₂ to give the title compound that is intended to be used to treat obesity, psychiatric and neurol. disorders.

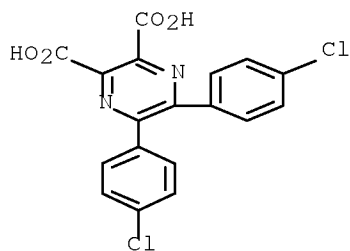
IT 810685-49-5P, 5,6-Bis(4-chlorophenyl)pyrazine-2,3-dicarboxylic acid 810685-51-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bis(chlorophenyl)piperidinylpyrazinecarboxamide derivative for treating obesity, psychiatric disorders, and neurol. disorders)

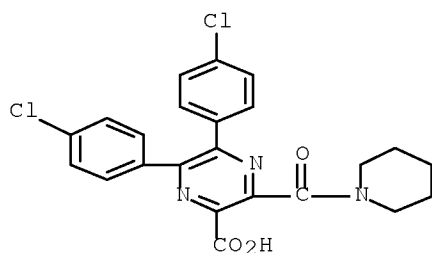
RN 810685-49-5 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)- (CA INDEX NAME)



RN 810685-51-9 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 5,6-bis(4-chlorophenyl)-3-(1-piperidinylcarbonyl)- (CA INDEX NAME)



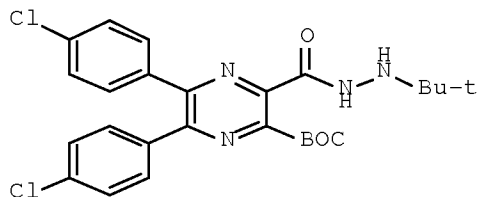
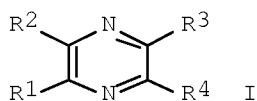
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:1127366 HCAPLUS Full-text
 DOCUMENT NUMBER: 142:56362
 TITLE: Preparation of 3-substituted
 5,6-diaryl-pyrazine-2-carboxamide and 2-sulfonamide
 derivatives as cannabinoid receptor 1 (CB1) modulators
 INVENTOR(S): Cheng, Leifeng
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
 SOURCE: PCT Int. Appl., 120 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004111034	A1	20041223	WO 2004-SE970	20040616
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004247616	A1	20041223	AU 2004-247616	20040616
CA 2527035	A1	20041223	CA 2004-2527035	20040616
EP 1638953	A1	20060329	EP 2004-749012	20040616
EP 1638953	B1	20080827		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004011508	A	20060725	BR 2004-11508	20040616
CN 1809554	A	20060726	CN 2004-80017200	20040616
JP 2006527771	T	20061207	JP 2006-517044	20040616
AT 406361	T	20080915	AT 2004-749012	20040616
NO 2005005919	A	20060216	NO 2005-5919	20051213
MX 2005PA13711	A	20060308	MX 2005-PA13711	20051215
KR 2006023152	A	20060313	KR 2005-724072	20051215
US 20070093484	A1	20070426	US 2005-560862	20051215 <--
PRIORITY APPLN. INFO.:			GB 2003-14057	A 20030618

OTHER SOURCE(S):
GI

MARPAT 142:56362



AB Title compds. I [wherein R1, R2 = independently (un)substituted Ph, thienyl, pyridinyl; R3 = X-Y-NR5R6; X = absent, CO, or SO2; Y = absent, NH optionally substituted by an alkyl group; R5, R6 = independently (un)substituted amino/alkyl, (CH2)r(phenyl)s, (un)saturated 5-8-membered heterocyclyl; R5 = H and R6 = defined above; or R5NR6 = (un)substituted (un)saturated 5-8-membered heterocyclyl; r = 0-4; s = 1 when r = 0, otherwise s = 1 or 2; R5NR6 = (un)substituted (un)saturated 5-8-membered heterocyclyl; R4 = (CH2)nCO2R7; n = 0-4; R7 = (un)substituted cycloalkyl/cyclo/alkyl, (CH2)nphenyl, saturated or partially unsatd. 5-8-membered heterocyclyl, CONH2 and derivs.; n = defined as above; and pharmaceutically acceptable salts thereof] were prepared as cannabinoid 1 (CB1) receptor modulators. For example, reacting 3-(tert-butoxycarbonyl)-5,6-bis(4-chlorophenyl)pyrazine-2-carboxylic acid (preparation given) with tert-butylhydrazine hydrochloride gave pyrazine II. I are active at the CB1 receptor (IC50 < 1 μM), most preferred compds. have IC50 < 200 nM. For instance, II exhibited an IC50 (hCB1) = 1.8 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of obesity, psychiatric and neurol. disorders (no data).

IT 810685-49-5P, 5,6-Bis(4-chlorophenyl)pyrazine-2,3-dicarboxylic acid 811436-88-1P, 3-(tert-Butoxycarbonyl)-5,6-bis(4-chlorophenyl)pyrazine-2-carboxylic acid 811441-05-1P, 5,6-Bis(4-chlorophenyl)-3-(ethoxycarbonyl)pyrazine-2-carboxylic acid 811441-55-1P, 5,6-Bis(4-methylphenyl)pyrazine-2,3-dicarboxylic acid 811441-57-3P, 3-(tert-Butoxycarbonyl)-5,6-bis(4-methylphenyl)pyrazine-2-carboxylic acid 811441-59-5P, 3-(Ethoxycarbonyl)-5,6-bis(4-methylphenyl)pyrazine-2-carboxylic acid 811441-81-3P, 5-(4-Chlorophenyl)-6-(4-methylphenyl)pyrazine-2,3-dicarboxylic acid 811441-84-6P, 3-(tert-Butoxycarbonyl)-5-(4-chlorophenyl)-6-(4-methylphenyl)pyrazine-2-carboxylic acid 811441-85-7P, 3-(tert-Butoxycarbonyl)-6-(4-chlorophenyl)-5-(4-methylphenyl)pyrazine-2-carboxylic acid 811441-88-0P, 5-(4-Chlorophenyl)-3-(ethoxycarbonyl)-6-(4-methylphenyl)pyrazine-2-carboxylic acid 811441-89-1P, 6-(4-Chlorophenyl)-3-(ethoxycarbonyl)-5-(4-methylphenyl)pyrazine-2-carboxylic acid

10/560862

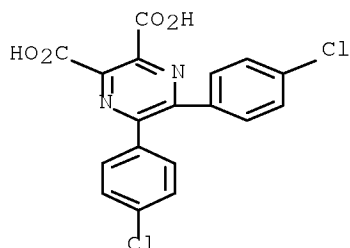
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 3-substituted 5,6-diarylpyrazine-2-carboxamide

and 2-sulfonamide derivs. as CB1 modulators)

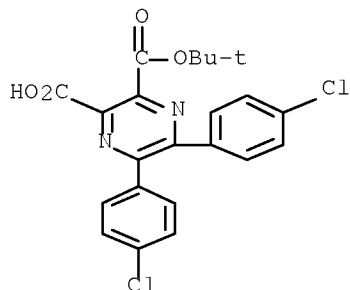
RN 810685-49-5 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)- (CA INDEX NAME)



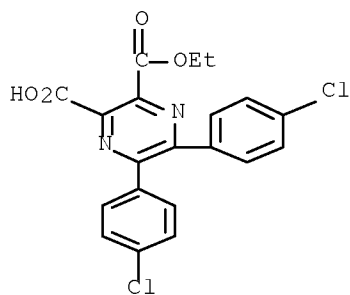
RN 811436-88-1 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)-, 2-(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 811441-05-1 HCAPLUS

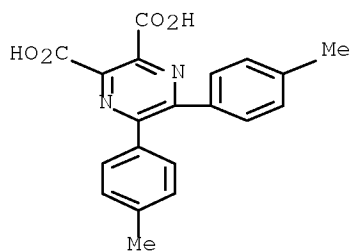
CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-chlorophenyl)-, 2-ethyl ester (CA INDEX NAME)



10/560862

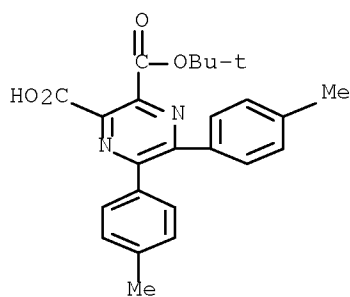
RN 811441-55-1 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-methylphenyl)- (CA INDEX NAME)



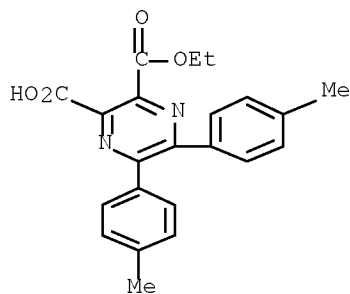
RN 811441-57-3 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-methylphenyl)-, 2-(1,1-dimethylethyl) ester (CA INDEX NAME)



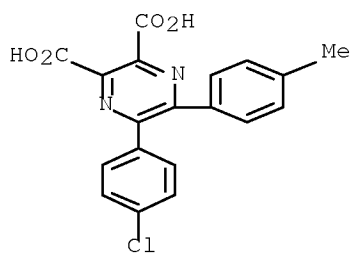
RN 811441-59-5 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-bis(4-methylphenyl)-, 2-ethyl ester (CA INDEX NAME)



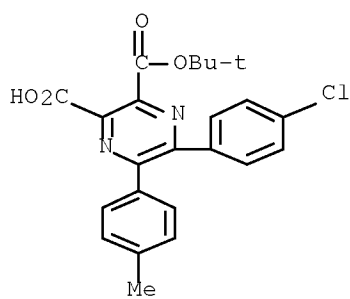
RN 811441-81-3 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5-(4-chlorophenyl)-6-(4-methylphenyl)- (CA INDEX NAME)



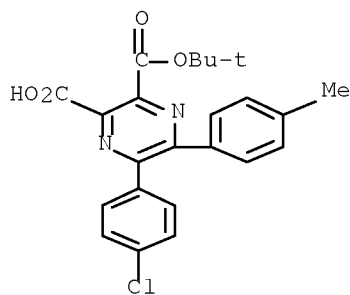
RN 811441-84-6 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5-(4-chlorophenyl)-6-(4-methylphenyl)-,
3-(1,1-dimethylethyl) ester (CA INDEX NAME)



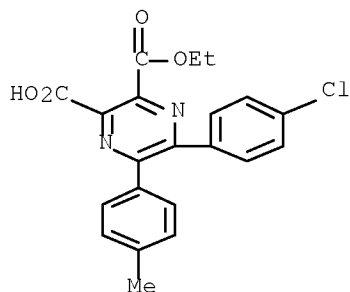
RN 811441-85-7 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5-(4-chlorophenyl)-6-(4-methylphenyl)-,
2-(1,1-dimethylethyl) ester (CA INDEX NAME)



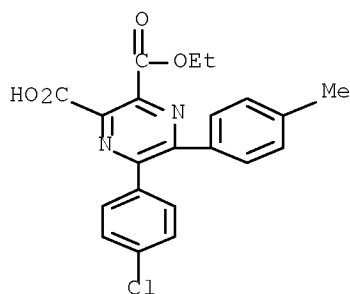
RN 811441-88-0 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5-(4-chlorophenyl)-6-(4-methylphenyl)-,
3-ethyl ester (CA INDEX NAME)



RN 811441-89-1 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5-(4-chlorophenyl)-6-(4-methylphenyl)-,
2-ethyl ester (CA INDEX NAME)



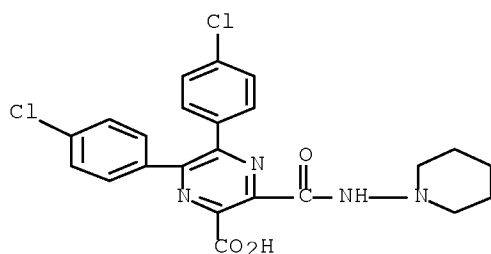
IT 811441-51-7, 5,6-Bis(4-chlorophenyl)-3-[[piperidin-1-yl]amino]carbonylpyrazine-2-carboxylic acid

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 3-substituted 5,6-diarylpyrazine-2-carboxamide and
2-sulfonamide derivs. as CB1 modulators)

RN 811441-51-7 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 5,6-bis(4-chlorophenyl)-3-[(1-piperidinylamino)carbonyl]- (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/560862

***** QUERY RESULTS *****

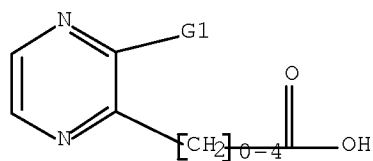
=> d his l24

(FILE 'HCAPLUS' ENTERED AT 10:35:32 ON 25 NOV 2008)

L24 5 S L21 NOT L23

=> d que l24

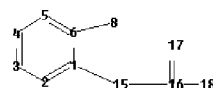
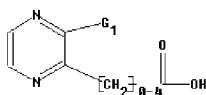
L9 STR



G1 [01], [02]

Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str



chain nodes :

8 9 10 11 15 16 17 18

ring nodes :

1 2 3 4 5 6

chain bonds :

1-15 6-8 9-10 15-16 16-17 16-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

6-8 9-10

exact bonds :

1-15 15-16

normalized bonds :

10/560862

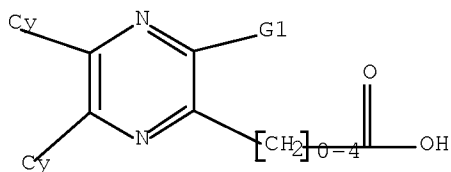
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18
isolated ring systems :
containing 1 :

G1:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS

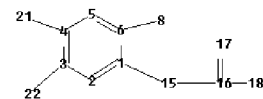
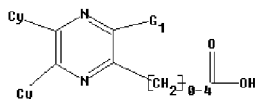
L11 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US20070093484/PN
L12 573 SEA FILE=REGISTRY SSS FUL L9
L18 STR



G1 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation:

Uploading L7.str



chain nodes :

8 9 10 11 15 16 17 18 21 22

ring nodes :

1 2 3 4 5 6

```

chain bonds :
1-15  3-22  4-21  6-8   9-10  15-16  16-17  16-18
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6
exact/norm bonds :
3-22  4-21  6-8   9-10
exact bonds :
1-15  15-16
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   16-17  16-18
isolated ring systems :
containing 1 :

```

```
G1:[*1],[*2]
```

```

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:Atom 22:Atom

```

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L20      22 SEA FILE=REGISTRY SUB=L12 SSS FUL L18
L21      9  SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20
L22     43 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "CHENG LEIFENG"/AU
L23      4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L22 AND L12) OR (L12 AND
      L11)
L24      5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 NOT L23

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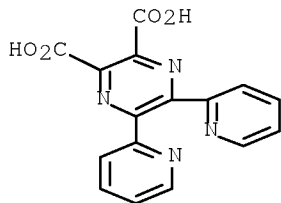
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L24  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:      2003:911996  HCAPLUS  Full-text
DOCUMENT NUMBER:      140:331239
TITLE:                  Dimensionality changes in crystalline complexes
                        induced by exposure to air: Solid-state studies using
                        single crystal and powder X-ray diffraction methods
AUTHOR(S):              Neels, Antonia; Alfonso, Montserrat; Mantero, Deborah
                        Gonzalez; Stoeckli-evans, Helen
CORPORATE SOURCE:       Institut de Chimie, Universite de Neuchatel,
                        Neuchatel, CH-2007, Switz.
SOURCE:                 Chimia (2003), 57(10), 619-622
                        CODEN: CHIMAD; ISSN: 0009-4293
PUBLISHER:              Swiss Chemical Society
DOCUMENT TYPE:          Journal
LANGUAGE:               English
AB    When they come into contact with air, coordination compds. can often change
      their appearance. For instance, the color of the compound can change as
      transparent crystals become opaque microcryst. solids. This visible
      transformation of the compound is frequently accompanied by structural
      modifications due to loss of solvent mols. or in the reverse case, the
      reaction with H2O from the air. Often, the dimensionality of the structures
      also varies and this aspect is demonstrated for three pairs of Cu(II)
      complexes (1-dimensional → 0-dimensional, 1-dimensional → 2-dimensional and
      3-dimensional → 2D). The complementary use of single crystal and powder x-
      ray diffraction methods is indispensable for the evaluation of these
      structural changes.

```

IT 374115-72-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for preparation of copper methylbis(pyridyl)pyrazine complex)
 RN 374115-72-7 HCAPLUS
 CN 2,3-Pyrazinedicarboxylic acid, 5,6-di-2-pyridinyl- (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 75
 IT 374115-72-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for preparation of copper methylbis(pyridyl)pyrazine complex)
 REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:749418 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:378975

TITLE: Hydrogen bonding in the inner-salt zwitterion and in two different charged forms of

5,6-bis(2-pyridyl)pyrazine-2,3-dicarboxylic acid

AUTHOR(S): Alfonso, Montserrat; Wang, Yi; Stoeckli-Evans, Helen

CORPORATE SOURCE: Institut de Chimie, Universite de Neuchatel,
 Neuchatel, CH-2007, Switz.

SOURCE: Acta Crystallographica, Section C: Crystal Structure
 Communications (2001), C57(10), 1184-1188
 CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 5,6-Bis(2-pyridyl)pyrazine-2,3-dicarboxylic acid exists as an inner-salt zwitterion, 3-carboxy-5-(2-pyridinio)-6-(2-pyridyl)pyrazine-2-carboxylate, (Ia), C₁₆H₁₀N₄O₄. The adjacent pyridine and pyridinium rings are almost coplanar due to the presence of an intramol. H bond involving the pyridine N atom and the NH H atom of the pyridinium group. In the crystal of (Ia), symmetry-related mols. are H bonded via the carboxylic acid OH group and one of the carboxylate O atoms to form a polymer, which exhibits a channel-type structure. In the HCl, HClO₄ and HPF₆ salts, 6-carboxy-5-carboxylatopyrazine-2,3-diyl-di-2-pyridinium chloride 2.25-hydrate, (II), C₁₆H₁₁N₄O₄·Cl·2.25H₂O, 6-carboxy-5-carboxylatopyrazine-2,3-diyl-di-2-pyridinium perchlorate trihydrate, (IIIa), C₁₆H₁₁N₄O₄·ClO₄·3H₂O, and 6-carboxy-5-carboxylatopyrazine-2,3-diyl-di-2-pyridinium hexafluorophosphate trihydrate, (IIIb), C₁₆H₁₁N₄O₄·PF₆·3H₂O, both pyridine rings are protonated. In the perchlorate form, and in the isomorphous hexafluorophosphate form, the mol. possesses C₂ symmetry, with has a sym. intramol. H bond involving the adjacent carboxylate and carboxylic acid substituents. In the crystals of the chloride and perchlorate (or hexafluorophosphate) salts, H-bonded polymers are formed

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which are three-dimensional and 1-dimensional, resp. Crystallog. data are given.

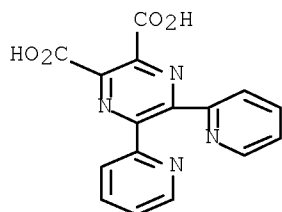
IT 374115-73-8 374115-74-9 374115-75-0

RL: PRP (Properties)

(crystal structure of)

RN 374115-73-8 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-di-2-pyridinyl-, hydrochloride, hydrate
(4:4:9) (CA INDEX NAME)



● HCl

● 9/4 H₂O

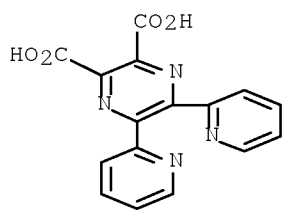
RN 374115-74-9 HCAPLUS

CN 2,3-Pyrazinedicarboxylic acid, 5,6-di-2-pyridinyl-, perchlorate, hydrate
(1:1:3) (CA INDEX NAME)

CM 1

CRN 374115-72-7

CMF C16 H10 N4 O4

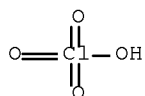


CM 2

CRN 7601-90-3

CMF C1 H O4

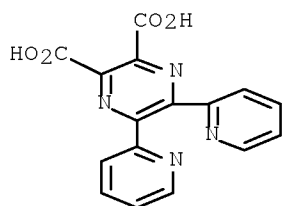
10/560862



RN 374115-75-0 HCAPLUS
 CN Phosphate(1-), hexafluoro-, hydrogen, compd. with
 5,6-di-2-pyridinyl-2,3-pyrazinedicarboxylic acid (1:1), trihydrate (9CI)
 (CA INDEX NAME)

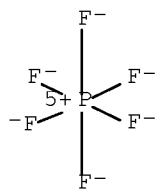
CM 1

CRN 374115-72-7
 CMF C16 H10 N4 O4

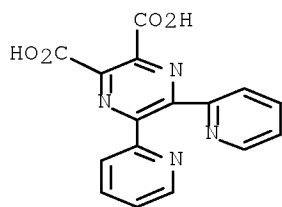


CM 2

CRN 16940-81-1
 CMF F6 P . H
 CCI CCS



IT 374115-72-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystal structure of inner-salt zwitterionic)
 RN 374115-72-7 HCAPLUS
 CN 2,3-Pyrazinedicarboxylic acid, 5,6-di-2-pyridinyl- (CA INDEX NAME)

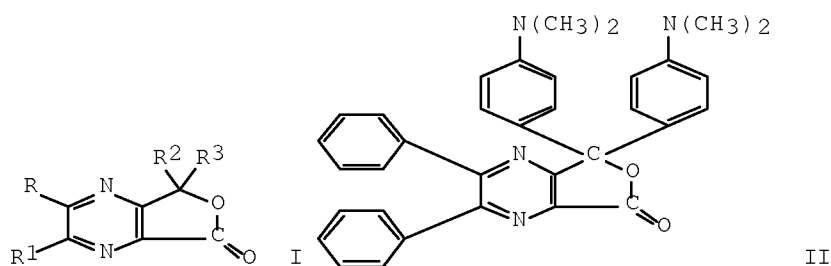


CC 75-8 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 28
 IT 374115-73-8 374115-74-9 374115-75-0
 RL: PRP (Properties)
 (crystal structure of)
 IT 374115-72-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystal structure of inner-salt zwitterionic)
 REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:111426 HCAPLUS Full-text
 DOCUMENT NUMBER: 106:111426
 ORIGINAL REFERENCE NO.: 106:18079a,18082a
 TITLE: Chromogenic compounds for pressure-sensitive and
 thermal copying processes
 INVENTOR(S): Hall, Nigel
 PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
 SOURCE: Eur. Pat. Appl., 52 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 192328	A1	19860827	EP 1986-300305	19860117
EP 192328	B1	19900509		
R: CH, DE, FR, GB, IT, LI				
JP 61195164	A	19860829	JP 1986-31036	19860217
PRIORITY APPLN. INFO.:			GB 1985-4631	A 19850222
OTHER SOURCE(S):	MARPAT 106:111426			

GI



AB Chromogenic pyrazine derivs. I [R, R¹ = H, alkenyl, alkoxy, aryl, etc. provided that R and R¹ are not H at the same time; R² and R³ = heterocyclic ring having aryl group annealed through a conjugated N linkage a homocyclic aryl group having substituent NR⁴R⁵; R⁴, R⁵ = H, R⁴ and R⁵ together with the N to which they are joined may form an heterocyclic ring provided R⁴ and R⁵ = H at the same time] are described for thermal recording materials and pressure-sensitive copying papers with improved lightfastness. Thus, a thermal recording paper was prepared by coating with a composition containing II and bisphenol A as developer to give green colored images with excellent lightfastness.

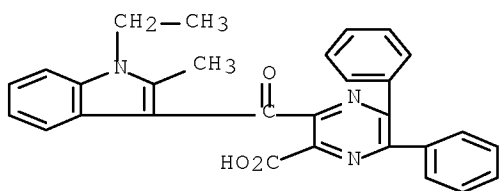
IT 105490-93-5P 105490-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of chromogenic pyrazine derivative)

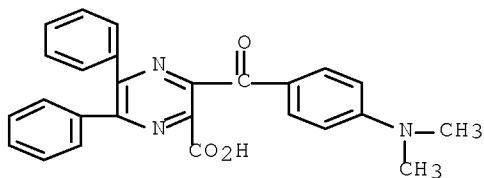
RN 105490-93-5 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 3-[(1-ethyl-2-methyl-1H-indol-3-yl)carbonyl]-5,6-diphenyl- (CA INDEX NAME)



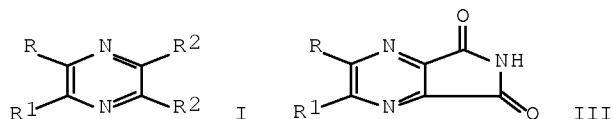
RN 105490-95-7 HCAPLUS

CN 2-Pyrazinecarboxylic acid, 3-[4-(dimethylamino)benzoyl]-5,6-diphenyl- (CA INDEX NAME)

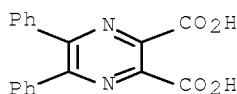


IC ICM C07D491-048
ICS B41M005-12
CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 28
IT 105490-93-5P 105490-94-6P 105490-95-7P 105490-96-8P
105490-97-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of chromogenic pyrazine derivative)

L24 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:68939 HCAPLUS Full-text
DOCUMENT NUMBER: 96:68939
ORIGINAL REFERENCE NO.: 96:11329a,11332a
TITLE: Synthesis of pyrazinedicarboximides from diaminomaleonitrile
AUTHOR(S): Tsuda, Tadataka; Fujishima, Katsuhiko; Ueda, Hiroo
CORPORATE SOURCE: Coll. Agric., Univ. Osaka Prefect., Osaka, 591, Japan
SOURCE: Agricultural and Biological Chemistry (1981), 45(9), 2129-30
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:68939
GI



AB Hydrolysis of pyrazines I (R = H, Me, Ph, 4-ClC6H4, 3,4-Cl2C6H3, 4-MeOC6H4; R1 = H, Me, Ph; R2 = CN), prepared from diaminomaleonitrile, followed by esterification gave I (R2 = CO2Me)(II). Amidn. of II with NH3 followed by intramol. cyclocondensation gave the title compds. (III). II (R = Ph, R1 = H, R2 = CO2Me) showed bactericidal activity superior to that of phenazine oxide.
IT 53954-53-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 53954-53-3 HCAPLUS
CN 2,3-Pyrazinedicarboxylic acid, 5,6-diphenyl- (CA INDEX NAME)



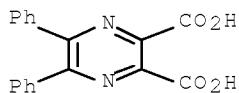
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5
 IT 89-01-0P 5521-60-8P 39784-64-0P 41110-52-5P ~~53954-53-3P~~
 80356-76-9P 80356-77-0P 80356-78-1P 80356-79-2P 80356-80-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and esterification of)

L24 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1975:58411 HCAPLUS Full-text
 DOCUMENT NUMBER: 82:58411
 ORIGINAL REFERENCE NO.: 82:9355a,9358a
 TITLE: Thermooxidative degradation of polyquinoxalines and
 related model compounds
 AUTHOR(S): Kane, James J.; Ghosh, Subrata; Conley, Robert T.
 CORPORATE SOURCE: Dep. Chem., Wright State Univ., Dayton, OH, USA
 SOURCE: Papers presented at [the] Meeting - American Chemical
 Society, Division of Organic Coatings and Plastics
 Chemistry (1973), 33(1), 466-73
 CODEN: ACOCAO; ISSN: 0096-512X
 DOCUMENT TYPE: Journal
 LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Solution oxidation by aqueous alkaline permanganate of model compds. for the
 poly(etherquinoxaline) (I) [52885-62-8] showed that the carbocyclic ring
 adjacent to the heterocyclic pyrazine ring was more susceptible to oxidation
 2-Phenylquinoxaline [5021-43-2] gave 2-phenylpyrazine-5,6-dicarboxylic acid
 [39784-64-0], and similarly, 2,3-diphenylpyrazine-5,6-dicarboxylic acid
 [53954-53-3] was prepared from 2,3-diphenylquinoxaline [1684-14-6],
 2,2',3,3'-tetraphenyl-6,6'-biquinoxaline [16111-01-6], 2,2',3,3'- tetraphenyl-
 6,6'-oxydiquinoxaline [16478-99-2], and 2,3-diphenylbenzo[g]quinoxaline
 [36305-72-3]. Pyrolytic oxidation of phenylquinoxalines gave products similar
 to those obtained from benzimides, suggesting that benzheterocyclic systems
 underwent oxidative degradation by similar mechanisms, with initial
 oxygenation of the carbocyclic ring adjacent to the heterocyclic one.
 Catalytic oxidation of the quinoxaline system involved oxygenated
 intermediates similar to pyrazine dicarboxylic acids. Nitrile absorptions
 were observed in ir spectra of oxidative pyrolysis products of I films.

IT ~~53954-53-3P~~
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, on oxidation of phenylquinoxalines)
 RN 53954-53-3 HCAPLUS
 CN 2,3-Pyrazinedicarboxylic acid, 5,6-diphenyl- (CA INDEX NAME)



CC 35-6 (Synthetic High Polymers)
 IT ~~53954-53-3P~~
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, on oxidation of phenylquinoxalines)

10/560862

***** SEARCH HISTORY *****

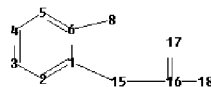
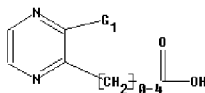
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FILE 'REGISTRY' ENTERED AT 10:10:25 ON 25 NOV 2008

L1 STRUCTURE UPLOADED
 D
L2 0 SEA SSS SAM L1
L3 STRUCTURE UPLOADED
 D
L4 0 SEA SSS SAM L3
L5 STRUCTURE UPLOADED
 D
L6 50 SEA SSS SAM L5
L7 STRUCTURE UPLOADED
 D
L8 50 SEA SSS SAM L7
L9 STRUCTURE UPLOADED
 D

Uploading L5.str



chain nodes :
8 9 10 11 15 16 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-15 6-8 9-10 15-16 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
6-8 9-10
exact bonds :
1-15 15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18
isolated ring systems :
containing 1 :

G1:[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS

L10 22 SEA SSS SAM L9

FILE 'HCAPLUS' ENTERED AT 10:20:26 ON 25 NOV 2008

L11 1 SEA ABB=ON PLU=ON US20070093484/PN
D SCAN TI

FILE 'STNGUIDE' ENTERED AT 10:22:09 ON 25 NOV 2008
D STAT QUE L9

FILE 'REGISTRY' ENTERED AT 10:23:40 ON 25 NOV 2008

L12 573 SEA SSS FUL L9
SAVE TEMP L12 JAI862REGL5/A
L13 STRUCTURE UPLOADED
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L14 1 SEA SUB=L12 SSS SAM L13
D SCAN

L15 4 SEA SUB=L12 SSS FUL L13
D SCAN

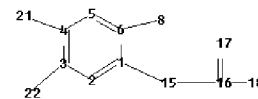
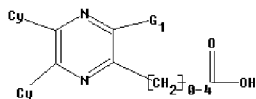
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L16 509 SEA ABB=ON PLU=ON L12
L17 95 SEA ABB=ON PLU=ON L16 AND PHARMAC?/SC, SX

FILE 'STNGUIDE' ENTERED AT 10:33:13 ON 25 NOV 2008

FILE 'REGISTRY' ENTERED AT 10:34:04 ON 25 NOV 2008
L18 STRUCTURE UPLOADED
D

Uploading L7.str



chain nodes :
8 9 10 11 15 16 17 18 21 22
ring nodes :
1 2 3 4 5 6
chain bonds :
1-15 3-22 4-21 6-8 9-10 15-16 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
3-22 4-21 6-8 9-10
exact bonds :
1-15 15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-18

isolated ring systems :
containing 1 :

G1:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:Atom 22:Atom

L19 3 SEA SUB=L12 SSS SAM L18
D SCAN

L20 22 SEA SUB=L12 SSS FUL L18
SAVE TEMP L20 JAI862REGL7/A

FILE 'HCAPLUS' ENTERED AT 10:35:32 ON 25 NOV 2008

L21 9 SEA ABB=ON PLU=ON L20
E CHENG LEIFENG/AU

L22 43 SEA ABB=ON PLU=ON "CHENG LEIFENG"/AU

L23 4 SEA ABB=ON PLU=ON (L22 AND L12) OR (L12 AND L11)

L24 5 SEA ABB=ON PLU=ON L21 NOT L23
SAVE TEMP L24 JAI862HCAP/A
SAVE TEMP L23 JAI862HCAIN/A

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D QUE L23

FILE 'HCAPLUS' ENTERED AT 10:39:45 ON 25 NOV 2008
D L23 1-4 IBIB ABS HITSTR

FILE 'STNGUIDE' ENTERED AT 10:39:47 ON 25 NOV 2008
D QUE L24

FILE 'HCAPLUS' ENTERED AT 10:40:14 ON 25 NOV 2008
D L24 1-5 IBIB ABS HITSTR HITIND

FILE 'STNGUIDE' ENTERED AT 10:40:16 ON 25 NOV 2008